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**DIFFUSION IN THE SURFACE LAYER OF THE
CONVECTIVE BOUNDARY LAYER**

FINAL REPORT

J. C. WEIL

JUNE 30, 1990

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1. Introduction

Dispersion in the planetary boundary layer (PBL) is important in a variety of problems including air pollution and obscurant cloud behavior in a battlefield environment. Dispersion is a stochastic phenomena caused by the random or stochastic nature of PBL turbulence, and the fluctuating concentration field often is as important as the mean field. Indeed, laboratory measurements show that the root-mean-square (rms) fluctuating concentration, σ_c , in plumes from continuous point sources can be 5 times greater than the ensemble-mean concentration C (Fackrell and Robins, 1982; Deardorff and Willis, 1988); a similar situation exists in smoke clouds (Hanna, 1984). Thus, σ_c as well as C must be estimated to assess the visibility limits of an obscurant cloud or the air quality effects of a pollution source.

Under a program sponsored by the U.S. Army Research Office (ARO), we have developed stochastic dispersion models for the C and σ_c fields due to a passive tracer source in the convective boundary layer (CBL), with the main aim of improving our understanding and predictability of dispersion in that layer. We focused on the CBL because: 1) the PBL is in a convective state a substantial fraction of the time ($\sim 30 - 40\%$), 2) the turbulence structure of the CBL is well documented (Wyngaard, 1988), and 3) laboratory data (Willis and Deardorff, 1976, 1978, 1981) and numerical results (Lamb, 1978) exist for testing models. Furthermore, dispersion in the CBL cannot be modeled by the standard statistical (Taylor, 1921) or eddy-diffusion theories because of the complications caused by the CBL turbulence—its vertical inhomogeneity, vertical velocity skewness, and large time scale.

The stochastic models developed in this program are Lagrangian and are thus a natural way to model dispersion, i.e., by following single particles or particle pairs through the turbulent flow given the Eulerian velocity statistics. The mean concentration is found from a "one-particle" model by computing the probability density function (p.d.f.) of particle position from the numerically-calculated particle trajectories. It is labeled "one-particle" because each particle is assumed to travel independently of the others. The "one-particle" model has progressed to the point of handling dispersion in inhomogeneous skewed turbulence with large time scales and thus can deal effectively with the complications in the CBL. The calculation of σ_c requires a "two-particle" model in which one tracks the simultaneous motion of two particles that start from some

random initial separation and arrive at the "same" place at the same time. The two-particle model is currently limited to homogeneous turbulence.

For the mean concentration, we developed a model for point and area sources with emphasis on the surface layer or lowest tenth of the CBL where the vertical inhomogeneity is strongest, but results have been generated for sources throughout the boundary layer. For concentration fluctuations, we developed a numerical code based on Thomson's (1990) recent model and have reproduced his key results. The current limitation of this model to homogeneous conditions means that it may only be applicable to elevated sources in the CBL, i.e., above the surface layer.

In the following sections, we briefly highlight the main results from this modeling program.

2. Mean Concentration Model

Dispersion is assumed to occur in a CBL with horizontally homogeneous but vertically inhomogeneous, stationary turbulence; the CBL is defined by $0 \leq z \leq h$, where z is the height above the surface and h is the depth of the layer. Only vertical dispersion is modeled, i.e., the vertical velocity and displacement of a particle, since the vertical and horizontal turbulence components are assumed to be independent. The mean wind U is taken to be uniform with z .

2.1. Single-Particle Model

Equations governing the vertical velocity w_L and height Z of a particle follow from Thomson's (1987) general model and have been used in Weil (1989, 1990a, 1990b). They are

$$dw_L = a(Z, w_L)dt + (C_0\epsilon)^{1/2}d\xi \quad (1)$$

$$dZ = w_L dt \quad (2)$$

where the first term $a(Z, w_L)$ on the right-hand-side of (1) is a deterministic velocity forcing function, the second term is the random forcing function, subscript L denotes a Lagrangian velocity, and t is time. In the second term, C_0 is an assumed universal constant taken as 2, ϵ is the ensemble-averaged turbulence dissipation rate, and $d\xi$ is a one-dimensional Gaussian random forcing with zero mean and variance dt .

The basis for choosing $a(Z, w_L)$ is discussed in Thomson (1987) and Weil (1990a) and requires an assumed form for the Eulerian p.d.f. of vertical velocity (w), $p_a(w)$. For

the inhomogeneous skewed turbulence of the CBL, p_a is assumed to be given by the sum of two Gaussian distributions. The parameters defining p_a are found by equating the zeroth through third moments of the assumed form with the specified moments in the CBL. The key moments are the second or velocity variance, $\sigma_w^2(z)$, and the third, $\overline{w^3}(z)$. The moments are prescribed by simple analytical functions which were chosen to be in broad agreement with laboratory experiments, field observations, and LES. Details of the $p_a(w)$, profiles of the velocity moments and ϵ , and the method of determining $a(Z, w_L)$ can be found in Weil (1989, 1990a).

For a point source, Eqs. (1) and (2) are numerically integrated to obtain $w_L(t)$ and $Z(t)$. The crosswind-integrated concentration (CWIC), C^y , downwind of a source can then be found from

$$C^y(x, z) = \frac{Q}{U} p_z \left(z - z_s, \frac{x - x_s}{U} \right) \quad (3)$$

(Weil, 1990a) where Q is the source emission rate, p_z is the p.d.f. of particle height at the downwind distance x , and subscript s denotes conditions at the source. p_z is found numerically from the particle trajectories with about 10^4 required to define a stable C^y value.

2.2. Point Source Results

One of the key tests of the model was a comparison of point source predictions with the laboratory experiments of Willis and Deardorff (1976, 1978, 1981), which were conducted for $z_s/h = 0.067, 0.24$, and 0.49 . We found that the isopleths of the CWIC in an $x - z$ plane were qualitatively similar to those in the experiments and for $z_s/h = 0.067$, they showed the familiar "lift-off" of the maximum CWIC from the surface. In addition, predictions of the mean particle displacement and the near-surface CWIC were in good agreement with the laboratory data both as a function of source height and downstream distance; these results were reported in Weil (1989).

In a further examination of the point source results, Weil (1989) investigated the sensitivity of the mean, $\langle Z \rangle$, and rms, $\langle Z^2 \rangle^{1/2}$, particle displacements and the CWIC field to the vertical velocity skewness $S = \overline{w^3}/\sigma_w^3$ with $S = 0$ or 0.6 . For sources in the middle of the CBL, $0.25 < z/h < 0.75$, the results showed that the differences between the skewed and nonskewed cases were small, and the trends were consistent with analytical results. The differences were most significant for sources at the boundaries. For the surface source, $\langle Z \rangle$ and $\langle Z^2 \rangle^{1/2}$ were both larger for $S = 0.6$ than for $S = 0$, whereas for $z_s = h$, the opposite was true.

A simple explanation for these results was given in terms of the w p.d.f. (Weil, 1990a). At the boundaries, particles are constrained to move away from the source with positive velocities if $z_s = 0$ and negative velocities if $z_s = h$. For $S > 0$, the velocity distribution is biased toward larger positive values and smaller negative ones than for $S = 0$ or Gaussian turbulence. Thus, in skewed turbulence particles originating at a surface source are transported upwards more rapidly than in Gaussian turbulence, and the converse is true for a source at h . This bias also explains the asymmetry in top-down and bottom-up diffusion from area sources in the CBL as discussed in Section 2.3.

In conjunction with this work, we conducted a systematic investigation of particle displacement statistics for sources in the surface layer ($z/h < 0.1$); preliminary results were reported in Weil (1990b) and a more complete paper is in preparation (Weil, 1990c). For a point source at the surface, $S = 0$, and a uniform ϵ with z , the mean and rms displacements exhibit the same dependence on downwind distance at short range ($X < 0.3$):

$$\frac{\langle Z \rangle}{h} = \alpha_1 X^{3/2}, \quad \frac{\langle Z^2 \rangle^{1/2}}{h} = \alpha_2 X^{3/2} \quad (4)$$

where X is a nondimensional distance (Willis and Deardorff, 1976),

$$X = \frac{w_* x}{Uh}, \quad (5)$$

and is the ratio of the travel time (x/U) to the large-eddy turnover time (h/w_*). The proportionality of the displacement heights to $X^{3/2}$ is consistent with Yaglom's (1972) similarity theory and results from the strong inhomogeneity in σ_w^2 in the surface layer, $\sigma_w^2 \propto z^{2/3}$. For $z_s/h \gtrsim 0.1$, $\langle Z^2 \rangle^{1/2} \propto X$ at short range ($X < 0.7$) which is consistent with Taylor's (1921) statistical theory for homogeneous turbulence; this is attributed to the quasi-homogeneity of turbulence for $z/h \gtrsim 0.1$.

For the surface source, two asymptotic models for $\langle Z \rangle$ were investigated: 1) an eddy-diffusion model with the diffusivity $K = \sigma_w^2 \tau$ which should be valid when $\tau = \sigma_w^2 / \epsilon \ll h/w_*$, and 2) a "trajectory" or "ballistic" model which is valid when $\tau \gg h/w_*$. The original motivation for the diffusion model was that $\tau \ll h/w_*$ very near the surface. However, this inequality breaks down at even modest heights and at $z/h \sim 0.1$, $\tau \simeq 0.5h/w_*$; i.e., it is not "small."

In the large τ limit, the equation for the Lagrangian velocity was solved analytically and integrated over time to yield $Z(t)$ (Weil, 1990b). $\langle Z(t) \rangle$ was found by averaging the $Z(t)$ expression over the p.d.f. of the random velocity at the source and resulted in

$\langle Z \rangle / h = 2.6X^{3/2}$. In the diffusion limit ($\epsilon \rightarrow \infty$), we found $\langle Z \rangle / h = 1.2(X/\epsilon_*)^{3/2}$ where $\epsilon_* = \epsilon h / w_*^3$. The interesting result was that the dependence of $\langle Z \rangle / h$ on X was the same in both τ limits, i.e., it was insensitive to ϵ_* . However, the coefficient α_1 was quite sensitive to ϵ_* being 2.6 as $\epsilon_* \rightarrow 0$ and $1.2\epsilon_*^{-3/2}$ as $\epsilon_* \rightarrow \infty$. Our numerical simulations supported these analytical results and yielded a smooth variation of α_1 with ϵ_* . For ϵ_* values (~ 1) typical of the surface layer, α_1 was not close to either asymptotic limit and would have to be obtained from the numerical simulations.

For a surface source, the simulations showed that the effect of a nearly constant, positive S was to increase α_1, α_2 relative to their values for $S = 0$ (Weil, 1989). This was caused by the bias in the w p.d.f. mentioned earlier. However, the $X^{3/2}$ dependence was retained for $S > 0$.

The model was extended to account for source momentum and buoyancy on the rise and growth of a continuous point-source plume. This was done by superposing the plume rise velocity, which was calculated from an integral model (Weil, 1988), and the random ambient velocity obtained from the stochastic model. A key new concept is that in a heated boundary layer the plume buoyancy flux decreases with time due to the increase in the mean CBL temperature with time. This is especially important for highly buoyant plumes that remain near the CBL top. The CWIC field and surface CWIC predicted by the model were in good agreement with laboratory simulations of highly buoyant plumes by Willis and Deardorff (1987). This work will be reported in a future publication.

2.3. Area Source Results

The stochastic model has also been used to study diffusion from area sources in the CBL and, in particular, to diagnose the asymmetry in bottom-up and top-down diffusion (Weil, 1990a), a phenomena first found in the LES of Moeng and Wyngaard (1984, 1989). Our analysis was simplified by considering the diffusion properties of hypothetical boundary layers with σ_w^2 and $\overline{w^3}$ profiles qualitatively similar to those in the CBL but with a uniform $\tau(z)$. The concentration field, $\overline{C}(z)$, due to a uniform area source was found by superposing the fields due to (crosswind) line sources distributed in the along-wind direction.

For inhomogeneous Gaussian turbulence, an asymmetry in diffusion patterns about the mid-plane of the boundary layer resulted from the vertical asymmetry in $\sigma_w(z)$. For $\tau \ll h/w_*$, this asymmetry was predictable from an eddy-diffusion model

with a z -dependent K since the effective $K(z)$ values determined from the simulations approached $K = \sigma_w^2 \tau$, the long-time limit of Taylor's (1921) theory. However, for $\tau w_*/h \geq 0.5$, K theory was inapplicable since $\partial \bar{C}/\partial z$ exhibited sign changes and K had singularities, indicating regions of a countergradient flux. The causes of the K model breakdown were the memory (i.e., large τ) and inhomogeneity of the turbulence which were measured through the dimensionless parameter $\tau \partial \sigma_w / \partial z$.

The simulations with inhomogeneous skewed turbulence showed that a positive S led to an asymmetry between bottom and top sources in both $\partial \bar{C}/\partial z$ and the effective K ; this was independent of the form of the variance profile, i.e., whether $\sigma_w^2(z)$ was symmetric about $h/2$ or not. Again, the asymmetry was caused by the bias in the w p.d.f. as discussed earlier.

Our simulations of top-down and bottom-up diffusion motivated a simple theoretical analysis of transport asymmetry in skewed turbulence (Wyngaard and Weil, 1989). A kinematic model for homogeneous skewed turbulence with a small time scale ($\ll h/w_*$) showed that the transport asymmetry was linked to the interaction of skewness with the scalar flux gradient. It showed that the K for bottom-up diffusion developed a singularity near $z = h$ whereas the K for the top-down case was positive and well-behaved. Stochastic model simulations showed that the asymmetry was sensitive to τ , with small effects for $\tau \sim 0.1h/w_*$ and large effects for $\tau \sim h/w_*$.

Another problem recently analyzed was the behavior of K and the dimensionless temperature gradient, ϕ_h , in the surface layer during very unstable conditions. Businger et al. (1971) showed that temperature measurements supported a $K \propto z^{3/2}$ behavior instead of $K \propto z^{4/3}$ as predicted by free-convection similarity theory. We analyzed this problem in the zero wind limit and proposed that the large convective eddies generate a thin shear layer near the surface in which $\epsilon \propto w_*^3/z$ and the σ_w at the surface is $\sigma_w \simeq 0.15w_*$, in analogy with a shear-driven surface layer; the ϵ behavior is consistent with the LES of Schmidt and Schumann (1989). With the assumed ϵ and σ_w , our stochastic model simulations showed that K in the surface layer behaved as $K \propto z^{3/2}$. For an assumed constant ϵ and a σ_w approaching zero at the surface (i.e., as in similarity theory), the simulations yielded $K \propto z^{4/3}$. Thus, the conceptual picture of the thin, convectively-driven shear layer along with the nonstandard ϵ and σ_w scalings seem to explain the findings of Businger et al. (1971). This work will be prepared for publication.

3. Concentration Fluctuation Model

3.1. Two-Particle Model

In a two-particle model, one calculates σ_c^2 at some point \mathbf{x} downwind of a source from

$$\sigma_c^2 = \langle c^2(\mathbf{x}, t) \rangle - C^2(\mathbf{x}, t) \quad (6)$$

where $\langle c^2 \rangle$ is the mean square concentration, and the bold-faced symbol denotes a vector. $\langle c^2 \rangle$ is found from the joint p.d.f. that two particles from some random initial separation arrive at the same point at the same time. This p.d.f. is found numerically from an ensemble of particle-pair trajectories.

We constructed a two-particle computer model based on Thomson's (1990) model and briefly summarize his general approach along with key results to demonstrate the capability of our code to reproduce his results.

Thomson proposed a three-dimensional model for two-particle dispersion in homogeneous turbulence and resolved many of the deficiencies of earlier two-particle models based on a one-dimensional formulation. His model is based on the same criteria used in the one-particle case and requires an assumed form of the velocity p.d.f.; in this case it is the two-point p.d.f. The model describes the evolution of the six-dimensional position (\tilde{X}) and velocity (\tilde{U}) arrays that define the two-particle system: $\tilde{X}(t) = (\tilde{x}_1(t), \tilde{x}_2(t))$ and $\tilde{U}(t) = (\tilde{u}_1(t), \tilde{u}_2(t))$, where the first three members of each array are the vector components of particle 1 (\tilde{x}_1 and \tilde{u}_1) and the second three are those of particle 2. The quantity (\tilde{X}, \tilde{U}) evolves according a Markov process with position and velocity given by stochastic equations similar to (1) and (2).

For homogeneous isotropic turbulence, the two-point velocity p.d.f. is assumed to be Gaussian with the velocity correlation tensor given by Batchelor (1953). The two scalar functions appearing in this tensor are found by: 1) requiring that the flow satisfy incompressibility, and 2) specifying the longitudinal correlation function, which describes the velocity correlation in the direction of the particle separation vector, $\tilde{\Delta}$. Thus, the important constraint of incompressibility is built into the two-particle model.

From his simulations, Thomson produced the correct rms two-particle separation (σ_Δ) with $\sigma_\Delta \propto t^{3/2}$ at short times ($t \ll \sigma_v^2/\epsilon$) and $\sigma_\Delta \propto t^{1/2}$ at long times ($t \gg \sigma_v^2/\epsilon$), i.e., consistent with inertial subrange theory (Batchelor, 1950). The model also gave the correct rms single particle displacement (σ_1): $\sigma_1 \propto t$ at short times and $\sigma_1 \propto t^{1/2}$ at long times in agreement with Taylor's (1921) theory. Figure 1a shows his results

for the above rms displacements along with σ_Σ which is the rms value of the random centroid position (Σ) of the two-particle system. The σ_v used in nondimensionalizing the displacement and time axes in Fig. 1 represents the rms turbulence velocity in this homogeneous, isotropic case; on the abscissa, s is the emission time and $t - s$ is the particle travel time.

Figure 1b shows the same rms displacements calculated from our two-particle code. As can be seen, the results are in excellent agreement with Thomson's and exhibit the same time variation discussed above.

The mean square concentration can be found using an approach given by Sawford (1983) and is based on an integral of p_Δ and p_Σ over the particle-pair source distribution; here, p_Δ and p_Σ represent the p.d.f.'s of the two-particle separation and centroid. We omit the details of the method but stress the importance of p_Δ and p_Σ in computing $\langle c^2 \rangle$.

Figure 2 shows p_Δ from Thomson's and our calculations for four dimensionless times $((t - s)/(\sigma_v^2/\epsilon))$, which are approximately the same in the two sets of calculations. As can be seen, our curves reproduce Thomson's results quite well. Note that p_Δ changes from a strongly peaked distribution at short times, $(t - s)/(\sigma_v^2/\epsilon) \ll 1$, to a Gaussian distribution at long times. In contrast, the p_Σ (not shown) is nearly Gaussian for all times; our p_Σ results also reproduce Thomson's. The integration over p_Δ and p_Σ to produce $\langle c^2 \rangle$ is being carried out and should be completed shortly.

3.2. Related Work on Concentration Fluctuations

In addition to stochastic modeling, we conducted two other investigations of concentration fluctuations. One analysis focused on the statistics of concentrations exceeding specified threshold levels and resulted in a publication (Kristensen et al., 1989). A second focused on the cumulative distribution function (c.d.f.) of concentration fluctuations from a point-source of nonbuoyant material in a laboratory-simulated CBL (Deardorff and Willis, 1988). We showed that the c.d.f. of c'/σ_c , where c' is the concentration fluctuation about C at any location and σ_c is the rms value at the same location, has a nearly self-similar shape over a broad range of distances. The measurements were made along the plume centerline at ground level. The self-similar shape has important and useful implications for modeling concentration fluctuations and the p.d.f. of c .

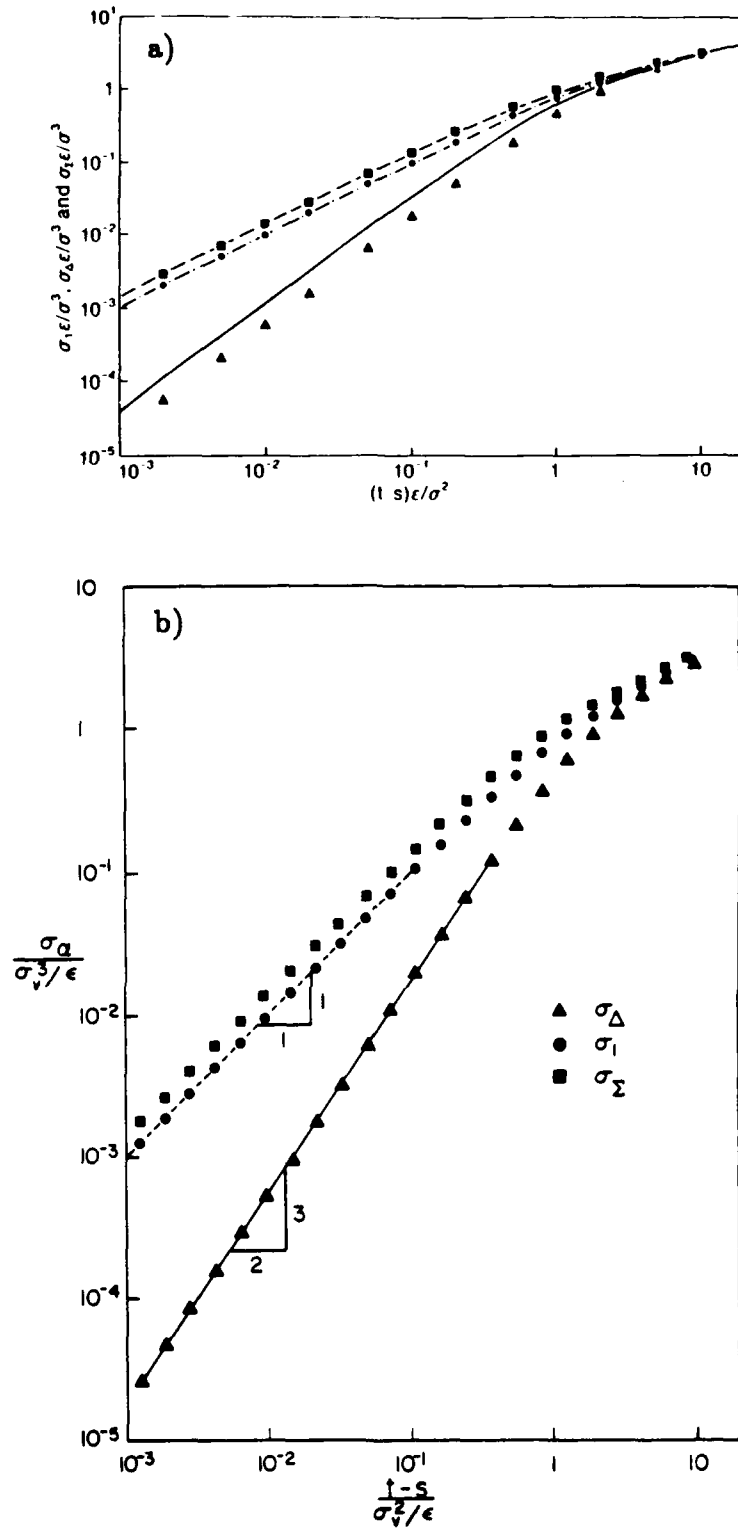


Figure 1. The root-mean-square values of particle-pair separation (σ_Δ), single-particle displacement (σ_1), and two-particle centroid displacement (σ_Σ) as a function of time: a) numerical results (points) computed by Thomson (1990) and analytical approximations (lines) from a simple model (see Thomson), and b) our numerical results. In b, α in σ_α represents Δ , 1, or Σ ; same plotting symbols used for σ_Δ , σ_1 , and σ_Σ in a and b (see b). Note difference in ordinate scales in a and b.

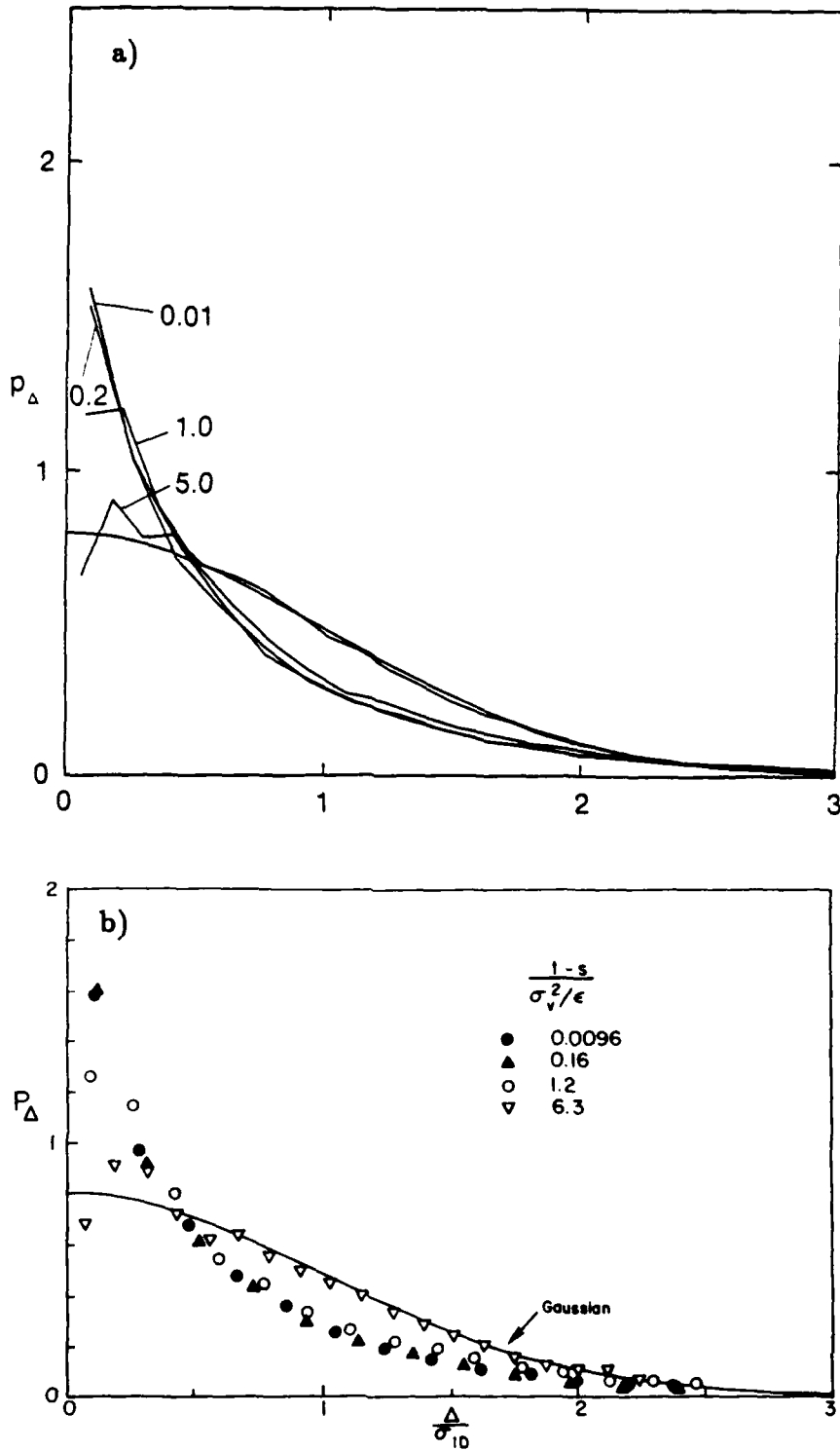


Figure 2. The probability density function of particle-pair separation as numerically computed: a) by Thomson (1990), and b) from our numerical two-particle code. The parameter in a is the dimensionless time $(t-s)/(\sigma_v^2/\epsilon)$ which is approximately the same in a and b. σ_{1D} is the effective one-dimensional value of the three-dimensional displacement (σ_Δ) in this homogeneous isotropic turbulence.

4. Publications Under this Program

Journal Articles and Published Proceedings

- Kristensen, L., J.C. Weil, and J.C. Wyngaard, 1989: Recurrence of high concentration values in a diffusing, fluctuating scalar field. *Bound.-Layer Meteor.*, **47**, 263-276.
- Weil, J.C., 1988: Atmospheric dispersion - observations and models. *Flow and Transport in the Natural Environment: Advances and Applications*, W.L. Steffen and O.T. Denmead, Eds., Springer-Verlag, 352-376.
- Weil, J.C., 1989: Stochastic modeling of dispersion in the convective boundary layer. *Air Pollution Modelling and Its Applications VII*, H. van Dop, Ed., Plenum, 437-449.
- Weil, J.C., 1990: A diagnosis of the asymmetry in top-down and bottom-up diffusion using a Lagrangian stochastic model. *J. Atmos. Sci.*, **47**, 501-515.
- Weil, J.C., 1990: Dispersion in the convective atmospheric surface layer. To be submitted to *Quart. J. Roy. Meteor. Soc.*
- Wyngaard, J.C., and J.C. Weil, 1989: Transport asymmetry in skewed turbulence. Submitted to *Phys. Fluids*.

Conference Proceedings

- Weil, J.C., 1988: Langevin model simulations of bottom-up and top-down dispersion in a nonhomogeneous turbulent boundary layer. *Preprints Eighth Symposium on Turbulence and Diffusion*, American Meteorological Society, Boston, 1-4.
- Weil, J.C., 1990: Dispersion limits in the convective surface layer. *Preprints Ninth Symposium on Turbulence and Diffusion*, American Meteorological Society, Boston, 344-347.

Report

- Weil, J.C., R.I. Sykes, A. Venkatram, and J.C. Wyngaard, 1988: The role of inherent uncertainty in evaluating dispersion models. Prepared by a special working group of the AMS/EPA Steering Committee on Air Quality Modeling. (This report is currently being shortened for a journal publication.)

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